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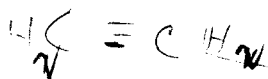
GREENBELT, MARYLAND

C_2 SWAN BANDS IN COMETS

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ABSTRACT

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The relative populations of the vibrational levels of the $X^3\Pi$ and $A^3\Pi$ electronic levels are calculated assuming the fluorescence mechanism. Pure vibrational transitions are taken into account by making a rough estimate of the magnetic-dipole transition probabilities. Both the approximate method, Rosseland's theory of cycles applied to a three-level molecule, and the accurate solution of the equations of statistical equilibrium for a 10-level molecule, give similar results. The excitation temperatures derived from these relative populations agree satisfactorily with the observations of the Swan bands by McKellar and Climenhaga (1953) for various sun-comet distances. Finally, an estimate is made of the infrared radiation, due to pure vibrational transitions, expected from a bright comet. The expected amount of radiation is small and will be difficult to detect.

Author

It is well known that the C_2 Swan bands observed in comets are excited by the mechanism of resonance fluorescence (Stawikowski and Swings 1960). Observations give excitation temperatures (defined by a Boltzmann distribution of the relative populations of vibrational levels of the $X^3\Pi$ ground electronic term) in the range $T_{ex} \approx 2000-3000^\circ$ at sun-comet distances of 0.48 to 1.40 a.u. (McKellar and Climenhaga 1953). Other cometary molecules such as CN , CH , NH and OH are observed to have much lower excitation temperatures, and this is understood qualitatively to be a consequence of spontaneous downward radiative transitions (vibrational and pure rotational) within the ground electronic terms of these molecules (Wurm 1936). In fact, quantitative calculations using estimated transition probabilities approximately match the observed excitation temperature (Hunaerts 1953, 1957). However C_2 has no permanent electric dipole moment, and the downward radiative transitions within the ground term are therefore forbidden, so that large populations occur in highly excited vibrational levels (Wurm 1936).

Houziaux (1960) has calculated the expected populations of successive vibrational levels in C_2 , taking account only of resonance fluorescence in the Swan bands, and assuming all transition probabilities within the ground $X^3\Pi$ term to be identically zero. However the calculations do not agree very well with observation in that the calculated excitation temperatures are higher than the observed excitation temperatures and furthermore vary considerably from one level to the next.

In fact, however, magnetic dipole transitions of the type $\Delta\Sigma = \pm 1$ can occur within the ground $X^3\Pi$ term of C_2 , since all the selection rules for this type of transition are fulfilled (Van Vleck 1934). We can see the approximate effect of these transitions by applying Rosseland's theory of cycles to a simplified 3 level molecule, taking the lowest levels 1 and 2 as successive vibrational levels of $X^3\Pi$, and the high level 3 as any vibrational level of the upper $A^3\Pi$ term that is connected by strong radiative transitions with both levels 1 and 2. Then the population ratio is (Ambartsumyan 1958).

$$\frac{n_2}{n_1} = W e^{-h\nu_{21}/kT} \frac{A_{31} e^{-h\nu_{32}/kT} + \frac{A_{21}}{A_{32}} (A_{31} + A_{32})}{W A_{31} e^{-h\nu_{32}/kT} + \frac{A_{21}}{A_{32}} (A_{31} + A_{32})} \quad (1)$$

$$\equiv e^{-h\nu_{21}/kT_{\text{ex}}}$$

where W is the dilution factor, T is the radiation temperature and T_{ex} is the observed temperature as defined above.

In a crude first approximation $A_{31} \approx A_{32} \gg A_{21}$ so if $W A_{31} \exp(-h\nu_{32}/kT) \gg A_{21}$, that is if the transition $2 \rightarrow 1$ is strongly forbidden, then $T_{\text{ex}} \approx T \approx 5730^\circ$. Alternatively, if $A_{31} \exp(-h\nu_{32}/kT) \ll A_{21}$, that is $2 \rightarrow 1$ can occur, then $W \exp(-h\nu_{21}/kT) \approx \exp(-h\nu_{21}/kT_{\text{ex}})$. For a comet at 1 a.u.

distance from the sun the geometrical dilution factor is $\underline{W} \approx 5 \times 10^{-6}$, $(\underline{h\nu}_{21}/\underline{kT}) \approx 0.4$, and this limit gives $\underline{T}_{\text{ex}} \approx 180^\circ$. The magnetic dipole transition probability is (Condon and Shortley 1951)

$$\underline{A}_{\text{vib}} = \frac{64\pi^4 \sigma^3}{3h} (a \underline{M} b)^2, \quad (2)$$

where $\sigma = 1618 \text{ cm}^{-1}$ is the wave number between successive vibrational levels, and $(a \underline{M} b)$ is the matrix element of the magnetic dipole moment, which we can crudely estimate to be 1 Bohr magneton. We thus roughly estimate $\underline{A}_{21} (= \underline{A}_{\text{vib}}) = 10^{-1} \text{ sec}^{-1}$, which is of the same order of magnitude as $\underline{W} \underline{A}_{31} \exp(-\underline{h\nu}_{32}/\underline{kT})$, but smaller than $\underline{A}_{31} \exp(-\underline{h\nu}_{32}/\underline{kT})$, since for the strongest transitions in the Swan bands $\underline{A}_{31} \approx 5 \times 10^6 \text{ sec}^{-1}$. Accordingly, we expect the calculated excitation temperature to be between the two limits above but closer to the first, that is, to be of the order of a few thousand degrees.

Therefore accurate calculations of the statistical equilibrium of cometary C_2 were made, taking into account the lowest 5 vibrational levels of the ground $\text{X } ^3\Pi$ term and also the lowest 5 vibrational levels of the upper $\text{A } ^3\Pi$ term.

The relative populations were obtained by solving the equations of statistical equilibrium. Equations similar to those of Houziaux (1960) were used, with the addition of pure vibrational transitions within the electronic terms. Only those pure vibrational transitions with $\Delta \underline{v} = \pm 1$ were considered. For completeness,

pure vibrational absorptions of solar infrared radiation were included, although they had negligible influence on the results. Following are the equations of statistical equilibrium, lower electronic term, $i=1, 5$:

$$n_{i-1} B_{i-1 \rightarrow i} \rho_{i-1 \rightarrow i}$$

$$-n_i (B_{i \rightarrow i-1} \rho_{i \rightarrow i-1} + A_{i \rightarrow i-1} + B_{i \rightarrow i+1} \rho_{i \rightarrow i+1} + \sum_{k=6}^{10} B_{ik} \rho_{ik}) \quad (3)$$

$$+ n_{i+1} (B_{i+1 \rightarrow i} \rho_{i+1 \rightarrow i} + A_{i+1 \rightarrow i}) + \sum_{k=6}^{10} n_k (B_{ki} \rho_{ki} + A_{ki}) = 0$$

upper electronic term $j=6, 10$:

$$n_{j-1} B_{j-1 \rightarrow j} \rho_{j-1 \rightarrow j}$$

$$-n_j [B_{j \rightarrow j-1} \rho_{j \rightarrow j-1} + A_{j \rightarrow j-1} + B_{j \rightarrow j+1} \rho_{j \rightarrow j+1} + \sum_{k=1}^5 (B_{jk} \rho_{jk} + A_{jk})] \quad (4)$$

$$+ n_{j+1} (B_{j+1 \rightarrow j} \rho_{j+1 \rightarrow j} + A_{j+1 \rightarrow j}) + \sum_{k=1}^5 n_k B_{kj} \rho_{kj} = 0$$

The notation is essentially the same as used by Houziaux (1960).

The same values of A_{vib} were used for all vibrational transitions of both upper and lower electronic terms. For the pure vibrational absorptions, all upper levels were assumed to absorb at $\lambda=5.70\mu$ while the lower absorbed at 6.18μ (these are wavelengths of the $\underline{v}=0$ to $\underline{v}=1$ transitions). The solar radiation at these wavelengths was obtained from Allen (1963). Values of the other parameters

used in equations (3) and (4) are listed in Table 1. The columns headed \underline{m} and \underline{n} refer to the subscripts used in equations (3) and (4). The transition probabilities were computed from the overlap integrals and the oscillator strength using the same values of these quantities as Houziaux (1960). The radiation densities were derived from the "mean monochromatic intensities" in Table 1 of Minnaert (1953). The transition probabilities and radiation densities computed here are slightly different from those of Houziaux, but either set of values gives essentially the same results.

The equations of statistical equilibrium were solved with the aid of an electronic computer. For comparison, we show in Table 2 the results of our work for the case with $\underline{A}_{\text{vib}} = 0$ and a sun-comet distance of 0.72 a.u. (which is probably the distance used by Houziaux) and Houziaux's results for the same case. We believe that there is some error in the latter. Table 3 shows the results for various values of $\underline{A}_{\text{vib}}$ and the sun-comet distance. In order to allow for uncertainties in the value of $\underline{A}_{\text{vib}}$, calculations were made with the assumed values $\underline{A}_{\text{vib}} = 1.0, 0.1$ and 0.01 sec^{-1} .

It can be seen that the results of Table 3 have the same behavior as the three-level case, i.e., decreasing vibrational temperature with increasing vibrational transition probability. It is also seen that transition probabilities between $\underline{A}_{\text{vib}} = 0.1$ and 1.0 sec^{-1} give excitation temperatures in the 2000-3000° range observed by McKellar and Climenhaga.

From the relative populations given in Table 3 it is also possible to estimate the expected infrared radiation of cometary C_2 . We will make this calculation for the (1,0) band of the lower electronic term, which occurs at 6.18μ . Both the earth-comet and sun-comet distances are taken as 1 a.u.

According to Wurm (1963), the number of C_2 molecules in the ground state of a typical bright comet is

$$N(C) \approx 6 \times 10^{32} \text{ molecules}$$

The luminosity in the (1,0) band is then given by the expression

$$L \approx \frac{N(v''=1)}{N(v''=0)} \cdot N(C_2) A_{vib} h\nu_{vib}$$

where $N(v''=1)/N(v''=0)$ is a relative population given in Table 3. With the assumption $A_{vib} = 0.1 \text{ sec}^{-1}$ we obtain $L \approx 9 \times 10^{18} \text{ ergs/sec}$, or a flux received at the earth, assuming the whole comet is in the field of the telescope, of about $3 \times 10^{-9} \text{ ergs/cm}^2 \text{ sec}$.

Rough calculations can be made as to the possibility of detecting this band. Assuming that the minimum power (i.e. Noise Equivalent Power) detectable by an infrared detector is about 10^{-11} watts ; and that 0.1 of the power incident on the telescope reaches the detector, then it would require a telescope diameter of several hundred inches to observe this band (even above the atmosphere). Clearly, detection of the infrared lines of C_2 are not to be expected.

In summary, then, with the estimated pure vibrational transition probabilities and the assumption of the fluorescence mechanism, we have been able to derive relative populations of a 10- level C_2 molecule. These results are in agreement with those suggested by a simplified 3- level molecule and with published observations of comets.

It has also been possible to predict the infrared emission expected from a bright comet. This emission seems too weak to be observed. Similar calculations need to be performed on other cometary molecules to predict their infrared spectra.

$2C^L$

REFERENCES

- Ambartsumyan, V. A. 1958, Theoretical Astrophysics
(London: Pergamon Press), p 416.
- Condon, E. U. and Shortley, G. H. 1951, The Theory of
Atomic Spectra (Cambridge: Cambridge University Press).
- Houziaux, L. 1960, Ann d'ap., 23, 1025.
- Hunaerts, J. 1953, Mem. Soc. R. Sci. Liege, 13, 59.
_____ 1957, Mem. Soc. R. Sci. Liege, 18, 82.
- McKellar, A., and Climenhaga, J. L. 1953 La Physique des
Cometes (Rept. of 4th Liege Symposium).
- Minnaert, M. 1953, The Sun (Chicago: University of Chicago
Press), p 92.
- Stawikowski, A., and Swings, P. 1960, Ann d'ap., 23, 585.
- Van Vleck, _____ 1934, Ap. J., 80, 161.
- Wurm, K. 1936, Handbuch der Physik, 7, 306.
_____ 1963, The Moon, Meteorites and Comets (Chicago:
University of Chicago Press)

TABLE 1
PARAMETERS USED IN THE EQUATIONS OF STATISTICAL EQUILIBRIUM

\underline{v}'	\underline{v}''	\underline{m}	\underline{n}	λ	$\underline{A}_{\underline{v}', \underline{v}''}$ sec ⁻¹	$\underline{B}_{\underline{v}', \underline{v}''}$ erg ⁻¹ cm ³ sec ⁻²	$\rho_{\underline{v}'', \underline{v}'}(0.72 \text{ a.u.})$ erg cm ⁻³ sec
0	0	6	1	5165	$6.36 \cdot 10^6$	$5.26 \cdot 10^{18}$	$1.135 \cdot 10^{-19}$
0	1	6	2	5635	$1.41 \cdot 10^6$	$1.52 \cdot 10^{18}$	1.258
0	2	6	3	6191	$2.12 \cdot 10^5$	$3.02 \cdot 10^{17}$	1.433
1	0	7	1	4737	$2.67 \cdot 10^6$	$1.71 \cdot 10^{18}$	1.020
1	1	7	2	5129	$3.23 \cdot 10^6$	$2.61 \cdot 10^{18}$	1.129
1	2	7	3	5585	$1.93 \cdot 10^6$	$2.02 \cdot 10^{18}$	1.263
1	3	7	4	6122	$4.60 \cdot 10^5$	$6.34 \cdot 10^{17}$	1.425
1	4	7	5	6764	$7.75 \cdot 10^4$	$1.44 \cdot 10^{17}$	1.530
2	0	8	1	4382	$3.42 \cdot 10^5$	$1.73 \cdot 10^{17}$	0.741
2	1	8	2	4715	$4.07 \cdot 10^6$	$2.56 \cdot 10^{18}$	1.009
2	2	8	3	5098	$1.47 \cdot 10^6$	$1.17 \cdot 10^{18}$	1.096
2	3	8	4	5540	$1.96 \cdot 10^6$	$2.02 \cdot 10^{18}$	1.223
2	4	8	5	6060	$6.68 \cdot 10^5$	$8.93 \cdot 10^{17}$	1.418
3	1	9	2	4371	$8.61 \cdot 10^5$	$4.32 \cdot 10^{17}$	0.737
3	2	9	3	4697	$4.68 \cdot 10^6$	$2.92 \cdot 10^{18}$	1.001
3	3	9	4	5071	$5.24 \cdot 10^5$	$4.10 \cdot 10^{17}$	1.119
3	4	9	5	5502	$1.89 \cdot 10^6$	$1.89 \cdot 10^{18}$	1.211
4	2	10	3	4365	$1.40 \cdot 10^6$	$6.98 \cdot 10^{17}$	0.734
4	3	10	4	4685	$4.98 \cdot 10^6$	$3.07 \cdot 10^{18}$	0.995

TABLE 2
RELATIVE POPULATIONS
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Lower Electronic Term		Upper Electronic Term	
$\underline{v''}$	$\underline{N}(\underline{v''})/\underline{N}(\underline{v''}=0)$	$\underline{v'}$	$\underline{N}(\underline{v'})/\underline{N}(\underline{v'}=0)$
1	0.69	0	$9.4 \cdot 10^{-8}$
2	0.48	1	6.4
3	0.33	2	4.3
4	0.23	3	2.9
		4	2.0

HOUZIAUX (1960)

Lower Electronic Term		Upper Electronic Term	
$\underline{v''}$	$\underline{N}(\underline{v''})/\underline{N}(\underline{v''}=0)$	$\underline{v'}$	$\underline{N}(\underline{v'})/\underline{N}(\underline{v'}=0)$
1	0.95	0	$1.0 \cdot 10^{-7}$
2	0.71	1	$8.7 \cdot 10^{-8}$
3	0.61	2	7.9
4	0.37	3	4.5
		4	6.1

TABLE 3

RELATIVE POPULATIONS AND BOLTZMANN TEMPERATURES

Lower Level			Upper Level	
$\underline{v''}$	$\underline{N(\underline{v''})}/\underline{N(\underline{v''}=0)}$	$\underline{T_{ex}}$	$\underline{v'}$	$\underline{N(\underline{v'})}/\underline{N(\underline{v'}=0)}$
$\underline{R} = 0.4 \text{ a.u.} \quad \underline{A_{vib}} = 1.0$				
1	0.39	25×10^2	1	0.50
2	0.22	31	2	0.25
3	0.12	33	3	0.14
4	0.06	32	4	0.09
$\underline{A_{vib}} = 0.1$				
1	0.65	53×10^2	1	0.65
2	0.44	56	2	0.42
3	0.29	56	3	0.28
4	0.20	56	4	0.19
$\underline{A_{vib}} = 0.01$				
1	0.69	63×10^2	1	0.68
2	0.48	62	2	0.45
3	0.33	61	3	0.31
4	0.23	62	4	0.21
$\underline{R} = 0.7 \text{ a.u.} \quad \underline{A_{vib}} = 1.0$				
1	0.20	14×10^2	1	0.39
2	0.09	19	2	0.13
3	0.04	21	3	0.06
4	0.01	21	4	0.03

TABLE 3 (Continued)

RELATIVE POPULATIONS AND BOLTZMANN TEMPERATURES

Lower Level			Upper Level	
$\underline{v''}$	$\underline{N(\underline{v''})}/\underline{N(\underline{v''}=0)}$	$\underline{T_{ex}}$	$\underline{v'}$	$\underline{N(\underline{v'})}/\underline{N(\underline{v'}=0)}$
$\underline{A_{vib}} = 0.1$				
1	0.56	40×10^2	1	0.60
2	0.36	46	2	0.36
3	0.24	48	3	0.23
4	0.14	46	4	0.16
$\underline{A_{vib}} = 0.01$				
1	0.68	60×10^2	1	0.67
2	0.47	61	2	0.45
3	0.32	60	3	0.30
4	0.22	60	4	0.20
$\underline{R} = 1.0 \text{ a.u.} \quad \underline{A_{vib}} = 1.0$				
1	0.11	11×10^2	1	0.34
2	0.04	15	2	0.08
3	0.01	16	3	0.03
4	0.004	17	4	0.01
$\underline{A_{vib}} = 0.1$				
1	0.47	31×10^2	1	0.55
2	0.28	37	2	0.30
3	0.17	39	3	0.18
4	0.09	38	4	0.12

TABLE 3 (Continued)

RELATIVE POPULATIONS AND BOLTZMANN TEMPERATURES

Lower Level			Upper Level	
$\underline{v''}$	$\underline{N(v'')}/\underline{N(v''=0)}$	$\underline{T_{ex}}$	$\underline{v'}$	$\underline{N(v')}/\underline{N(v'=0)}$
$\underline{A_{vib}} = 0.01$				
1	0.66	57×10^2	1	0.66
2	0.45	58	2	0.43
3	0.30	58	3	0.29
4	0.21	58	4	0.20
$\underline{R} = 1.4 \text{ a.u.} \quad \underline{A_{vib}} = 1.0$				
1	0.06	8×10^2	1	0.31
2	0.02	12	2	0.05
3	0.006	14	3	0.01
4	0.002	14	4	0.006
$\underline{A_{vib}} = 0.1$				
1	0.35	22×10^2	1	0.48
2	0.19	28	2	0.22
3	0.11	31	3	0.12
4	0.05	30	4	0.08
$\underline{A_{vib}} = 0.01$				
1	0.63	51×10^2	1	0.65
2	0.43	55	2	0.41
3	0.29	55	3	0.28
4	0.20	57	4	0.19